Equation of State Developments in T-1

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The latest release of the SESAME library was performed on April 7, 2004. The release contains new tables for the following materials: copper, aluminum, deuterium, butane, hexane, propane, He-3, and two d-He-3 50/50 mixtures. The new tables for these materials introduce eleven new material numbers. In addition, 72 new subtables were added. The release was verified and validated under Los Alamos National Laboratory (LANL) guidelines.

The new deuterium Equation of State (EOS) in the library is a retrofit done to match the diamond anvil room temperature isotherm and the Hugoniot obtained by the Sandia National Laboratories effort on the Z machine.

Analysis of the High Explosive EOS created by Sam Shaw (T-14) was performed to study the viability of extending the EOS over the standard SESAME temperature and density range while preserving his work to machine accuracy. After performing the analysis, we then completed two different extensions of these various EOS.

We produced five different EOS mixes to assist the work of the WBWG, which includes members from the Thermonuclear Applications Group (X-2) and the Primary Design and Assessment Group (X-4) in the Applied Physics Division.

We have assessed the EOS of various isotopes of LiH. This work was stimulated by questions raised by one of our users who noted that we have several such EOS and that the quality of most of them is questionable. (For example, some do not approach the ideal gas limit correctly.) We have compared diamond anvil data and shock data to all previous EOS and have produced a new EOS This work was completed in Quarter 1 of FY 2005.

An important direction in EOS research has been to improve the treatment of materials undergoing phase transitions. Work in T-1 has improved the microscopic theory, as well as algorithms for data analysis and dynamic simulations for such materials. A recent collaboration with experimentalists in other LANL divisions and Sandia has elucidated the EOS, phase diagram, and kinetics of Zr. A single EOS and kinetic model is able to accurately simulate the phase transition under shock wave and isentropic compression loading.

The current EOS for Be was called into question with the finding in the open literature of electronic structure results and diamond anvil data. To clarify this situation, we are performing density functional theory (DFT) calculations aimed at refining the EOS. Our preliminary results for the average phonon frequency led to a Grüneisen parameter in good agreement with our current EOS, but the results point to some improvements. If the minor differences between our DFT results and the earlier value remain with higher-accuracy calculations, they will be incorporated into a more accurate EOS.

The EOS experimental data set for Sn is fairly extensive, including information from efforts at Los Alamos and elsewhere on the melting curve and temperatures for release isentropes. To evaluate this data and provide direction to these experimental efforts, we have reexamined with care our current EOS for Sn and found it satisfactory but at odds with this data. We are now doing more detailed calculations to firm up our opinion. It is important to determine if there are problems with the experiments.

We have continued our work to extend the CCW methods for constructing EOS to the entire temperature and density range required for SESAME tables. We have determined how to extend the nuclear contribution to the free energy to very high temperatures, well beyond the liquid regime, and we have argued that the electron excitation-nuclear motion contribution, usually neglected at low temperatures, is also negligible at very high temperatures ($T \geq 100\ T_m$).

We calculated the adiabatic and non-adiabatic contributions to the free energy of metals due to the electron-phonon interaction at temperatures between 0 and 1.5 times the melting temperature. We considered different metals and found the zero temperature value of the non-adiabatic contribution for each, which had not been calculated previously. We also determined the crossover temperature between the adiabatic and non-adiabatic contribution for each metal and found that it is at rather high temperatures but below melting.

The Vibration-Transit Theory recently developed in our group has been applied to the study of the dynamic response of liquids, as experimentally observed in inelastic neutron scattering and inelastic x-ray scattering. We have calculated the dynamic structure factor for sodium from the theory and from molecular dynamics simulation for a simple monatomic liquid, a model for sodium. Once more we have found support for the validity of the theory. We have been able to establish the fundamental role of atomic vibrations in single random configurations in determining the essential character of the Brillouin peak in the dynamic structure factor. Further developments of the theory regarding the role of transits are underway.

We have worked on validation and verification of the T-1 EOS computer codes GRIZZLY and OpenSesame by: (1) developing test suites for both GRIZZLY and OpenSesame and comparing the results generated by running on several platforms, (2) analyzing the causes of the different results generated by running on different platform and improving the numeric methods in OpenSesame to minimize these differences, (To this end, the rational interpolator and the method of finding zeros of a function were changed. Also, iterative calls to the root finder replaced an unstable double binary/double Newton's method.), (3) improving code documentation (http://opensesame.lanl.gov), (4) placing all code, test suites, and documentation under version control, and (5) modernizing GRIZZLY so that it ports easily to new platforms.

We have improved the capabilities of OpenSesame by: (1) adding an isobar plotting capability, and (2) adding melt models, shear modulus models, the Morse models, the Virial match model, and the Rose models.

We have made periodic releases to the user community of OpenSesame and GRIZZLY.

We participated in the Isentropic Compression Experiments (ICE) workshop at Sandia and provided theoretical support. The group is continually working on establishing a stronger collaboration effort with the Z machine and gas gun efforts at Sandia.

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